

# Exact Eigenvalues and Eigenfunctions of the Hulthén Potential in the PT–Symmetry for Any Angular Momentum

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# Abstract

The Schrödinger equation with the PT-symmetric Hulthén potential is solved exactly by taking into account effect of the centrifugal barrier for any  $l$ -state. Eigenfunctions are obtained in terms of the Jacobi polynomials. The Nikiforov-Uvarov method is used in the computations. Our numerical results are in good agreement with the ones obtained before.

Keywords: Energy Eigenvalues and Eigenfunctions; Hulthén potential; PT-symmetry; Nikiforov-Uvarov Method.

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## I. INTRODUCTION

The Hulthén potential [1] is a short-range potential in physics. The potential form is

$$V^{(H)}(r) = -Ze^2\delta\frac{e^{-\delta r}}{1 - e^{-\delta r}}, \quad (1)$$

where  $Z$  is a constant and  $\delta$  is the screening parameter. If the potential is used for atoms, the  $Z$  is identified with the atomic number. This potential is a special case of the Eckart potential [2], which has been widely used in several branches of physics and its bound states and scattering properties have been investigated by a variety of techniques [3].

The radial Schrödinger equation for the Hulthén potential can be solved analytically only for s-states ( $l = 0$ ) [1,4,5]. For  $l \neq 0$ , a number of methods have been used to find bound-state energies numerically [3,6-16] and analytically [17,18]. In this context, we present in this letter a Nikiforov-Uvarov method [19] within the frame of PT-symmetric quantum mechanics [20-27] to solve analytically the Hulthén superpotential partner  $(l+1)$ th member for non-zero angular momentum states given by Ref.[18]:

$$V_{(l+1)}^{(H)}(r) = -Ze^2\delta\left[1 - l(l+1)\frac{\hbar^2\delta}{2mZe^2}\right]\frac{e^{-\delta r}}{1 - e^{-\delta r}} + \frac{\hbar^2\delta^2}{2m}l(l+1)\frac{e^{-2\delta r}}{(1 - e^{-\delta r})^2}, \quad l = 0, 1, 2, \dots \quad (2)$$

which is for s-states is not shape invariant [28] and leads to the usual Hulthén potential (1). On the other hand, Eq.(2) can be rearranged as

$$V_{eff}^{(H)}(r) = V_{(l+1)}(r) = -Ze^2\delta\frac{e^{-\delta r}}{1-e^{-\delta r}} + \frac{l(l+1)\hbar^2\delta^2}{2m}\frac{e^{-\delta r}}{(1-e^{-\delta r})^2}, \quad (3)$$

which is well-known as the approximate Hulthén effective potential introduced by Greene and Aldrich [29].<sup>1</sup> It is of much concern to see that for small values of  $\delta$ , Eq.(3) becomes the effective Coulomb potential given by

$$V_{eff}^{(H)}(r, \delta \approx 0) \rightarrow V_{eff}^{(C)} = -\frac{Ze^2}{r} + \frac{l(l+1)\hbar^2}{2mr^2}. \quad (4)$$

In the case of Coulomb potential, the Hamiltonian corresponds to the addition of an appropriate barrier potential and the so-called degeneracy is recovered as a natural consequence [18]. At small values of  $r$ , the Hulthén potential, behaves like a Coulomb potential whereas for large values of  $r$  it decreases exponentially so its capacity for bound state is smaller than the Coulomb potential. The coulomb problem is analytically solvable for all energies and angular momenta. Because of the similarity and points of contrast mentioned above between Coulomb and Hulthén potentials, it may be of much interest to use the Hulthén superpotential partner, Eq.(2), to generate their eigenvalues and eigenfunctions in the framework of the PT-symmetric quantum mechanics by employing Nikiforov-Uvarov (NU) method. The outline of the paper is as follows: In section II, we solve the Schrödinger equation SE with Hulthén superpotential for its energy eigenvalues and eigenfunctions. In section III, we consider the  $l = 0$  and  $l \neq 0$  cases and compare with the other works and methods. Finally, section IV is for our conclusions.

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<sup>1</sup>In Ref.[30] the Hulthén effective potential is taken as  $V_{eff}^{(H)}(r) = -\delta\frac{e^{-\delta r}}{1-e^{-\delta r}} + \frac{l(l+1)}{2}\left(\delta\frac{e^{-\delta r}}{1-e^{-\delta r}}\right)^2$  in atomic units.

## II. POLYNOMIAL SOLUTION OF THE HULTHÉN POTENTIAL

The NU method provides us an exact solution of non-relativistic SE for certain kind of potentials [19]. The method is based upon the solutions of general second order linear differential equation with special orthogonal functions [31]. For a given real or complex potentials, the SE in one dimension, which is a PT-symmetric equation, is reduced to a generalized equation of hypergeometric type with an appropriate  $s = s(x)$  coordinate transformation. Thus, it takes the form:

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0, \quad (5)$$

where  $\sigma(s)$  and  $\tilde{\sigma}(s)$  are polynomials, at most of second-degree, and  $\tilde{\tau}(s)$  is of a first-degree polynomial. To find a particular solution for SE by separation of variables, we use the transformation given by

$$\psi(s) = \phi(s)y(s). \quad (6)$$

This reduces SE into an equation of hypergeometric type:

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0, \quad (7)$$

where  $\phi(s)$  is found to satisfy the condition  $\phi'(s)/\phi(s) = \pi(s)/\sigma(s)$ . Further,  $y(s)$  is the hypergeometric type function whose polynomial solutions are given by Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s)\rho(s)], \quad (8)$$

where  $B_n$  is a normalizing constant and the weight function  $\rho(s)$  must satisfy the condition [19]

$$(\sigma(s)\rho(s))' = \tau(s)\rho(s). \quad (9)$$

The function  $\pi(s)$  and the parameter  $\lambda$  required for this method are defined by

$$\pi(s) = \frac{\sigma'(s) - \tilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)}, \quad (10)$$

and

$$\lambda = k + \pi'(s). \quad (11)$$

Here,  $\pi(s)$  is a polynomial with the parameter  $s$  and the determination of  $k$  is the essential point in the calculation of  $\pi(s)$ . Thus, for the determination of  $k$ , the discriminant under the square root is being set equal to zero and the resulting second-order polynomial has to be solved for its roots  $k_{1,2}$ . Hence, a new eigenvalue equation for the SE becomes

$$\lambda_n + n\tau'(s) + \frac{n(n-1)}{2}\sigma''(s) = 0, \quad (n = 0, 1, 2, \dots) \quad (12)$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s), \quad (13)$$

and it will have a negative derivative.

Now, we follow Ref.[32], by rewritting Eq.(2) in a quite simple form as

$$V(r) = -V_1 \frac{e^{-\delta r}}{1 - e^{-\delta r}} + V_2 \left( \frac{e^{-\delta r}}{1 - e^{-\delta r}} \right)^2, \quad (14)$$

with

$$V_1 = Ze^2\delta \left[ 1 - l(l+1) \frac{\hbar^2\delta}{2mZe^2} \right] \text{ and } V_2 = \frac{\hbar^2\delta^2}{2m}l(l+1). \quad (15)$$

Therefore, using the separation of variables

$$\psi(\mathbf{r}) = \frac{1}{r}R(r)Y(\theta, \phi), \quad (16)$$

we may write the radial part of SE for all angular momentum states as

$$-\frac{\hbar^2}{2m} \frac{d^2 R(r)}{dr^2} + \left( V(r) + \frac{l(l+1)\hbar^2}{2mr^2} \right) R(r) = ER(r). \quad (17)$$

On the other hand, the one-dimensional counterpart of Eq.(17) can be written, in a PT-symmetric form, as

$$R''(x) + \frac{2m}{\hbar^2} \left[ E + \frac{V_1 e^{-\delta x}}{1 - e^{-\delta x}} - \frac{V_2 e^{-2\delta x}}{(1 - e^{-\delta x})^2} \right] R(x) = 0, \quad (18)$$

and with the assignment  $s = e^{-\delta x}$ , then it becomes

$$\frac{d^2 R(s)}{ds^2} + \frac{1}{s} \frac{dR(s)}{ds} + \frac{2m}{\hbar^2 \delta^2 s^2} \left[ E + \frac{V_1 s}{1-s} - \frac{V_2 s^2}{(1-s)^2} \right] R(s) = 0, \quad (19)$$

and also introducing the given dimensionless parameters

$$\epsilon = -\frac{2mE}{\hbar^2 \delta^2} > 0 \quad (E < 0), \quad \beta = \frac{2mV_1}{\hbar^2 \delta^2} \quad (\beta > 0), \quad \gamma = \frac{2mV_2}{\hbar^2 \delta^2} \quad (\gamma > 0), \quad (20)$$

finally it leads into the following simple hypergeometric form given by

$$\frac{d^2 R(s)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{dR(s)}{ds} + \frac{1}{[s(1-s)]^2} \times \left[ -(\epsilon + \beta + \gamma) s^2 + (2\epsilon + \beta) s - \epsilon \right] R(s) = 0. \quad (21)$$

Hence, comparing the last equation with the generalized hypergeometric type, Eq.(5), we obtain the associated polynomials as

$$\tilde{\tau}(s) = 1 - s, \quad \sigma(s) = s(1 - s), \quad \tilde{\sigma}(s) = -(\epsilon + \beta + \gamma) s^2 + (2\epsilon + \beta) s - \epsilon. \quad (22)$$

When these polynomials are substituted into Eq.(10), with  $\sigma'(s) = 1 - 2s$ , we obtain

$$\pi(s) = -\frac{s}{2} \pm \frac{1}{2} \sqrt{(1 + 4\epsilon + 4\beta + 4\gamma + 4k) s^2 - 4(\beta + 2\epsilon + k) s + 4\epsilon}. \quad (23)$$

Further, the discriminant of the upper expression under the square root has to be set equal to zero. Therefore, it becomes

$$\Delta = [4(\beta + 2\epsilon + k)]^2 - 4 \times 4\epsilon(1 + 4\epsilon + 4\beta + 4\gamma + 4k) = 0. \quad (24)$$

Solving Eq.(24) for the constant  $k$ , we get the double roots as  $k_{+,-} = -\beta \pm \sqrt{\epsilon(1 + 4\gamma)}$ , and substituting these values for each  $k$  into Eq.(23), we obtain

$$\pi(s) = -\frac{s}{2} \pm \frac{1}{2} \begin{cases} \left[ (2\sqrt{\epsilon} - \sqrt{1 + 4\gamma}) s - 2\sqrt{\epsilon} \right]; & \text{for } k_+ = -\beta + \sqrt{\epsilon(1 + 4\gamma)}, \\ \left[ (2\sqrt{\epsilon} + \sqrt{1 + 4\gamma}) s - 2\sqrt{\epsilon} \right]; & \text{for } k_- = -\beta - \sqrt{\epsilon(1 + 4\gamma)}. \end{cases} \quad (25)$$

Making the following choice for the polynomial  $\pi(s)$  as

$$\pi(s) = -\frac{s}{2} - \frac{1}{2} \left[ (2\sqrt{\epsilon} + \sqrt{1 + 4\gamma}) s - 2\sqrt{\epsilon} \right], \quad (26)$$

gives the function:

$$\tau(s) = 1 - 2s - \left[ \left( 2\sqrt{\epsilon} + \sqrt{1 + 4\gamma} \right) s - 2\sqrt{\epsilon} \right], \quad (27)$$

which has a negative derivative of the form  $\tau(s) = - \left( 2 + 2\sqrt{\epsilon} + \sqrt{1 + 4\gamma} \right)$ . Thus, from Eq.(11) and Eq.(12), we find

$$\lambda = -\beta - \frac{1}{2} \left( 1 + 2\sqrt{\epsilon} \right) \left( 1 + \sqrt{1 + 4\gamma} \right), \quad (28)$$

and

$$\lambda_n = - \left( 2 + 2\sqrt{\epsilon} + \sqrt{1 + 4\gamma} \right) n - n(n - 1). \quad (29)$$

After setting  $\lambda_n = \lambda$  and solving for  $\epsilon$ , we find:

$$\epsilon_n = \left[ \frac{1 + 2n}{2} - \frac{(n(n + 1) + \beta)}{1 + 2n + \sqrt{1 + 4\gamma}} \right]^2. \quad (30)$$

which is exactly Eq.(26) in Ref.[32] for the deformed Woods-Saxon potential if one lets  $q = -1$  and  $a = 1/\delta$ . Therefore, substituting the values of  $\epsilon$ ,  $\beta$  and  $\gamma$  into Eq.(30), one can immediately determine the Hulthén's exact energy eigenvalues  $E_{n,l+1}$  as

$$E_{n,l+1}^{(H)} = -\frac{\hbar^2 \delta^2}{2m} \left[ \frac{1 + 2n}{2} - \frac{\left( n(n + 1) + \frac{2mV_1}{\hbar^2 \delta^2} \right)}{1 + 2n + \sqrt{1 + \frac{8mV_2}{\hbar^2 \delta^2}}} \right]^2, \quad 0 \leq n < \infty. \quad (31)$$

Therefore, substituting, Eq.(15) into Eq.(31), one gets

$$E_{n,l+1}^{(H)} = -\frac{\hbar^2}{2m} \left[ \frac{(me^2 Z / \hbar^2)}{n + l + 1} - \frac{(n + l + 1)}{2} \delta \right]^2, \quad 0 \leq n < \infty. \quad (32)$$

for  $l + 1$  Hulthén superpotential. Following Ref.[32], in atomic units ( $\hbar = m = c = e = 1$ ) and for  $Z = 1$ , Eq.(32) turns out to be

$$E_{n,l+1}^{(H)} = -\frac{1}{2} \left[ \frac{1}{n + l + 1} - \frac{(n + l + 1)}{2} \delta \right]^2, \quad 0 \leq n < \infty, \quad l = 0, 1, 2, \dots \quad (33)$$

or

$$E_{\bar{n},l}^{(H)} = -\frac{1}{2} \left[ \frac{1}{\bar{n} + l} - \frac{\bar{n} + l}{2} \delta \right]^2, \quad \bar{n} = n + 1, \quad l = 0, 1, 2, \dots \quad (34)$$

which is exactly the same result obtained by other works (cf. e.g., Ref.[33], Eq.(78)) if  $l$  is set equal to zero. The above equation indicates that we deal with a family of Hulthén potentials.<sup>2</sup> Equation (32) agrees with Eq.(5) in Ref.[18] for  $l \neq 0$  case, and Eq.(11) in

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<sup>2</sup>The critical screening  $\delta_c$ , at which  $E_n = 0$ , is defined, in atomic units, by  $\delta_c = 2/(n + l + 1)^2$ .

Ref.[30] for  $l = 0$  case. Of course, it is clear that by imposing appropriate changes in the parameters  $\delta$  and  $V_1$ , the index  $n$  describes the quantization for the bound energy states. In addition, if the parameter  $V_2$  in Eq.(31) is adjusted to zero, solution reduces to the form obtained for the standard Hulthén potential without a barrier term (cf. e.g., Eqs.(14) and (15) with  $l = 0$  case).

Let us now find the corresponding wavefunctions. Applying the NU method, the polynomial solutions of the hypergeometric function  $y(s)$  depends on the determination of weight function  $\rho(s)$  which is found to be

$$\rho(s) = (1-s)^{\eta-1} s^{2\sqrt{\epsilon}}; \quad \eta = 1 + \sqrt{1+4\gamma}. \quad (35)$$

Substituting into the Rodrigues relation given in Eq.(8), the eigenfunctions are obtained in the following form

$$y_{n,q}(s) = C_n (1-s)^{-(\eta-1)} s^{-2\sqrt{\epsilon}} \frac{d^n}{ds^n} \left[ (1-s)^{n+\eta-1} s^{n+2\sqrt{\epsilon}} \right], \quad (36)$$

where  $C_n$  stands for the normalization constant and its value is  $1/n!$ . The polynomial solutions of  $y_n(s)$  are expressed in terms of Jacobi Polynomials, which is one of the classical orthogonal polynomials, with weight function  $(1-s)^{\eta-1} s^{2\sqrt{\epsilon}}$  in the closed interval  $[0, 1]$ , yielding  $A_n P_n^{(2\sqrt{\epsilon}, \eta-1)}(1-2s)$  [31]. Finally, the other part of the wave function in Eq.(6) is found to be

$$\phi(s) = (1-s)^\mu s^{\sqrt{\epsilon}}, \quad \mu = \eta/2. \quad (37)$$

Combining the Jacobi polynomials and  $\phi(s)$  in Eq.(36), the s-wave functions ( $l = 0$ ) could be determined as

$$R_n(s) = D_n s^{\sqrt{\epsilon}} (1-s)^\mu P_n^{(2\sqrt{\epsilon}, \eta-1)}(1-2s), \quad (38)$$

with  $s = e^{-\delta x}$  and  $D_n$  is a new normalization constant.

### III. CONCLUSIONS

The exact solutions of the radial SE for the Hulthén potential with the angular momentum  $l = 0$  and  $l \neq 0$  are found by using NU method. Eigenvalues and eigenfunctions obtained from the real form of the potential are computed. Therefore, the wave functions are physical and energy eigenvalues are in good agreement with the results obtained by the other methods. In this regard, Figure 1 shows the variation of the Hulthén potential with  $r$  for  $S$ -,  $P$ -, and  $D$ -states. Figure 2 plots the variation of the Hulthén potential with  $r$  for the  $S$ -state with various screening parameters  $\delta = 0.002, 0.01$  and  $0.1$ . Figures 3 and 4 show the variation of the energy eigenvalues with respect to the quantum number  $n$  for  $S$ - and  $P$ -states with the a chosen values of screening parameter  $\delta = 0.002, 0.05$  and  $0.2$ , respectively. On the other hand, Table 1 shows the bound energy eigenvalues of the Hulthén potential as a function of  $\delta$  for various quantum numbers of  $S$ -state. These results are compared with other works [11,33]. Further, the bound energy eigenvalues as a function of  $\delta$  for the states  $2p$  ( $n = 0, l = 1$ ) and  $3d$  ( $n = 1, l = 1$ ) [30] are given in Table 2. Comparison of our results with numerical data of Refs.[3,30] is also given. However, since the form of the potential used in our work has a different form than the potential form used by Ref.[30] in Eq. (14), we have to add a perturbation term,  $\Delta E$ , to our calculations in order to substitute the small differences in [18]. Better results have been obtained for the  $2p$  state for small values of  $\delta$  since the effective potential (3) becomes closer to the original Hulthén potential (1) and for small  $l$  the contribution of this angular momentum term in potential is also small. Therefore, if all the parameters of potential remain purely real, it is clear that all bound energies  $E_n$  with  $n \geq 0$  represent a negative energy spectrum [32]. We also point out that the exact results obtained for the Hulthén potential may have some interesting applications in the study of different quantum mechanical systems and atomic physics.

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## FIGURES

FIG. 1. Variation of the Hulthén potential as a function  $r$ . The curves are shown for screening parameter  $\delta = 0.2$  for the  $S$ -,  $P$ -, and  $D$ -states.

FIG. 2. Variation of the Hulthén potential as a function  $r$ . The curves are shown for  $S$ -state with various values of the screening parameter  $\delta = 0.002, 0.01$  and  $0.1$ .

FIG. 3. The variation of the energy eigenvalues with respect to the quantum number  $n$ . The curves shown are for  $S$ -state with various values of the screening parameters  $\delta = 0.002, 0.05$  and  $0.2$ .

FIG. 4. The variation of the energy eigenvalues with respect to the quantum number  $n$ . The curves shown are for  $P$ -state with the same screening parameters as in Figure 3.

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# TABLES

TABLE I. The  $S$ -states energy eigenvalues of the Hulthén potential for several values of screening parameter  $\delta$ .

$n$	$-E_n[11]$	$-\overline{E}_n[33]$	$-E_{exact}$	Our work
$\delta = 0.002$				
1	0.4990005	0.4990005	0.4990005	0.4990005
2	0.1240020	0.1240020	0.1240020	0.1240020
3	0.0545601	0.0545601	0.0545601	0.0545601
4	0.0302580	0.0302580	0.0302580	0.0302580
5		0.0012500		0.0190125
$\delta = 0.01$				
1	0.4950125	0.4950125	0.4950125	0.4950125
2	0.1200500	0.1200500	0.1200500	0.1200500
3	0.0506681	0.0506681	0.0506681	0.0506681
4	0.0264501	0.0264500	0.0264500	0.0264500
5	0.0153128	0.0153125	0.0153125	0.0153125
$\delta = 0.05$				
1	0.4753125	0.4753125	0.4753125	0.4753125
2	0.1012503	0.1012500	0.1012500	0.1012500
3	0.0333746	0.0333681	0.0333681	0.0333681
4	0.0113035	0.0112500	0.0112500	0.0112500
5		0.0028125		0.0028125
$\delta = 0.2$				
1	0.4049962	0.4050000	0.4050000	0.4050000
2	0.0450856	0.0450000	0.0450000	0.0450000
3		0.0005556		0.0005556
4		0.0112500		0.0112500

TABLE II. Energy eigenvalues as a function of the screening parameter  $\delta$  for the states  $2p$  and

$3d$ .

State	$\delta$	$-E_{n,l}$ [3] <sup>a</sup>	$-E_{n,l}$ [30] <sup>b</sup>	Our work <sup>c</sup>
$2p$	0.025	0.112760	0.1127605	0.1128125
	0.050	0.101042	0.1010425	0.1012500
	0.075	0.089845	0.0898478	0.0903125
	0.100	0.079170	0.0791794	0.0800000
	0.150	0.059495	0.0594415	0.0612500
	0.200	0.041792	0.0418860	0.0450000
$3d$	0.025	0.043601	0.0437069	0.0437590
	0.050	0.032748	0.331645	0.0333681
	0.075	0.023010	0.0239397	0.0243837
	0.100	0.014433	0.0160537	0.0168056

<sup>a</sup>Variational method.

<sup>b</sup>Numerical integration.

<sup>c</sup>The small difference in results is because the potential form used by Ref.[30] for  $l \neq 0$  part is different than our form.







